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Materials Stability

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Introduction

The NNSA laboratories have interest in advancing the fundamental computation tools that will elucidate the physics of materials aging and stability. The specific materials and degradation processes of interest to the national laboratories are diverse and provide a broad field of research. To drive this research toward impact it will be important to develop science based understanding of materials aging that can inform continuum level models for predictive simulation of performance during the product lifecycle. Linking the manufacturing processes to the resulting material state, how the material ages and how the material performs is an enormous technical challenge. To meet this challenge, it will be necessary for researchers to develop new computational tools and algorithms that can probe fundamental mechanisms that could not otherwise be explained or observed. Application of novel computation techniques to bridging spatial and temporal domains will require novel experimental techniques and accelerated aging methods for model validation.

Materials and Degradation Processes of Interest

To fully understand materials aging and performance it is often necessary to understand the bulk material behavior as well as the material interfaces and surfaces. Bulk materials of interest to the national laboratories are extremely broad including: metals, polymers, energetic materials, adhesives, catalyst, ceramics, glasses, lubricants, desiccants, nano-particles, and composites. Potential degradation modes of interest include, but are not limited to, corrosion, diffusion, microstructural evolution, thermo-mechanical fatigue, tribological wear, adhesive delamination, destabilization of explosives, oxidation of o-rings/silicones/foams, and materials fracture.

More recent interest around microsystems and nano-materials, that allow enhanced functionality have caused increased interest in developing models that describe materials aging at surface/interfaces. Research of interest would provide fundamental understanding of the microstructural mechanisms and topographical features that control mechanical, electrical, and tribological behavior of materials and how they age. Of particular interest is the relationship between microstructure, fine scale geometric features, and materials performance properties such as strength, fatigue resistance, and nano-tribological behavior and how these evolve when exposure to various environments. Understanding solid-solid interfaces in determining the reliability of materials systems, emphasizing the dynamics of grain boundaries, microstructure evolution, and interfacial fracture are of interest. To develop this fundamental understanding will require the bridging of spatial and temporal domains that will challenge current computation capabilities.

Given the extensive list of materials and mechanism of interest, the priority is to develop novel methods, tools and diagnostics that can be applied to the general study of materials aging.

Linking Manufacturing to Material Aging

Material properties and performance are determined by composition and structure, where the latter includes molecular and/or lattice structure, defect populations, and polycrystalline microstructure. These in turn are determined by processing, both in manufacturing and through aging, the inevitable alteration occurring over the product lifecycle. The performance and reliability of a product is inherently dependent on the properties and performance of the constituent materials. Research of materials aging and stability will provide fundamental understanding of how well these materials meet the demands of their designed application. The objective of research in materials aging will be to develop and apply science-based modeling and simulation capabilities to advance our understanding of the explicit mechanisms governing material behavior in a wide range of conditions.

Novel Methodology Development

In order to probe fundamental mechanisms of materials stability and aging, it is expected that a range of fundamental physics codes such as molecular dynamics and density functional theory, will find application. Improvements in these methods and critical algorithms will likely be required to address the range of challenges described. Transforming these fundamental understandings into continuum level descriptions that can predicting aging mechanism will require novel approaches. These problems challenge the start of the art in bridging temporal and spatial domains, requiring new computation approaches.

Validation and Verification (V&V)

For all the above interests, validation and verification are also required. Verification is the
process of determining that a computer simulation correctly represents the conceptual model and its solution – i.e., that the simulation approach has solved the problem correctly. Validation is the process of determining the degree to which a computer simulation is an accurate representation of the real world – i.e., that the simulation approach has solved the correct problem. Synchronization of code validation and experimental programs is a high priority of the V&V program and will be critical to a successful alliance program.

It is challenging to design accelerated aging experiments that accurately represent realistic aging scenarios. As such, developing fundamental approaches and tools, that can provide insight around materials aging mechanisms and the associated change in the materials response is a ripe area of research. Developing these advanced diagnostics or methodologies for model validation will be part of this activity.

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